# Clustering

## (unsupervised learning)

John Joseph Valletta

University of Exeter, Penryn Campus, UK

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www.exeter.ac.uk/as/rdp/

# Overview

- What is clustering?
- Major types of clustering methods
- $k$-means clustering
- Agglomerative hierarchical clustering
- Gaussian mixture models
- How do we determine the correct number of clusters?

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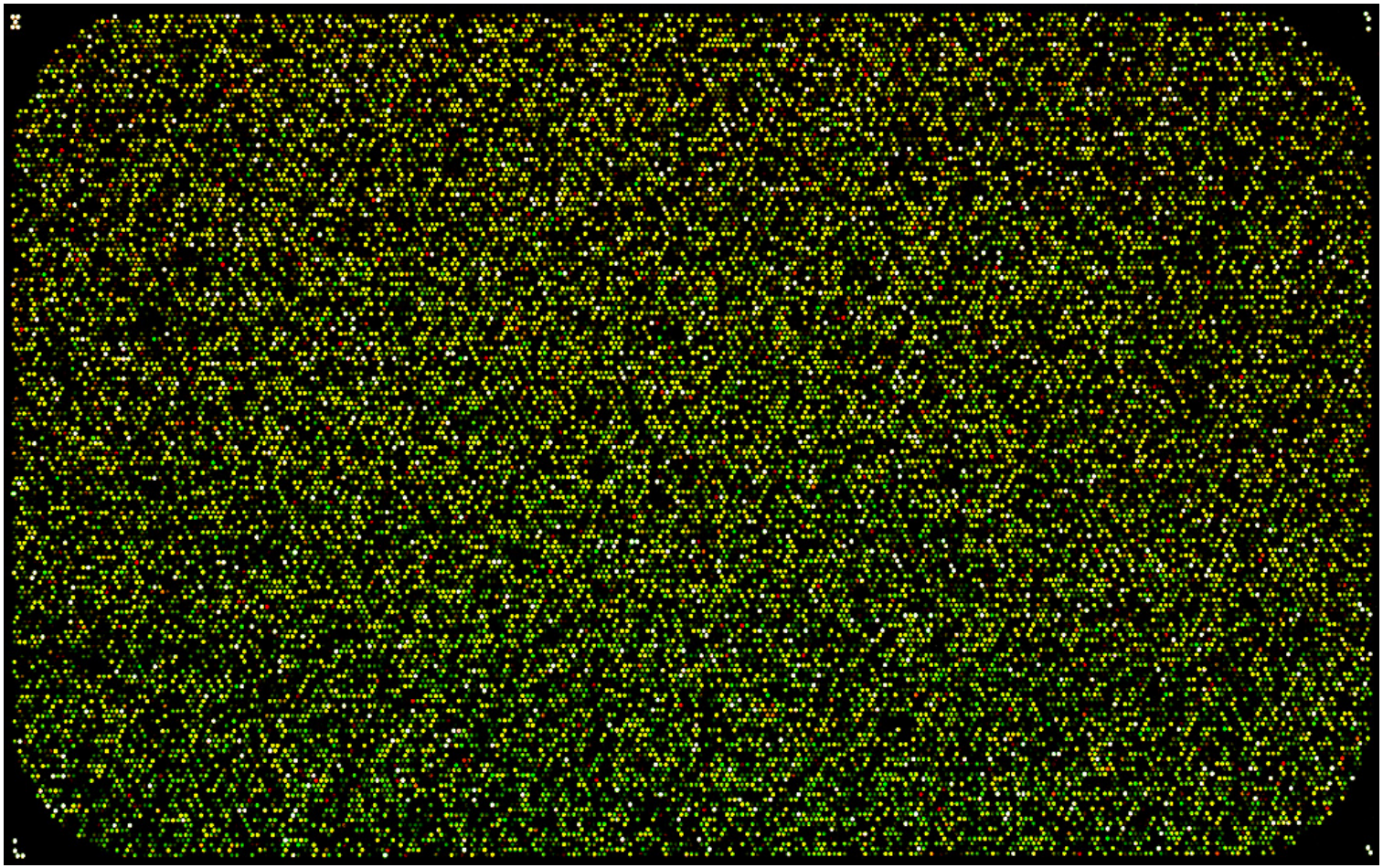
# What's the problem?

Well, it's driven by your data, e.g which of these genes are co-regulated?



We want to find some underlying structure in the data $\rightarrow$ **Clustering**

# What's the problem?

| | |
|---|---|
| Gene expression: | discovering co-regulated genes |
| Biological systematics: | finding organisms sharing similar attributes |
| Computer vision: | segmenting a digital image for object recognition |
| Epidemiology: | identifying geographical clusters of diseases |
| Medical imaging: | differentiating between tissues |
| Mathematical chemistry: | grouping compounds by topological indices |

**Clustering is particularly useful in applications where labelling the data is very time consuming/expensive**

# What is clustering?

## Formal definition

Identifying homogeneous and well separated groups of data points (features) by some similarity measure

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The process of stereotyping your data
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e.g *these* are round(ish) faces, *these* are short(ish) people

## But how many groups?

An unsolved problem. Issue lies in the subjectivity of the word **similar** and its mathematical definition

# Are they similar?

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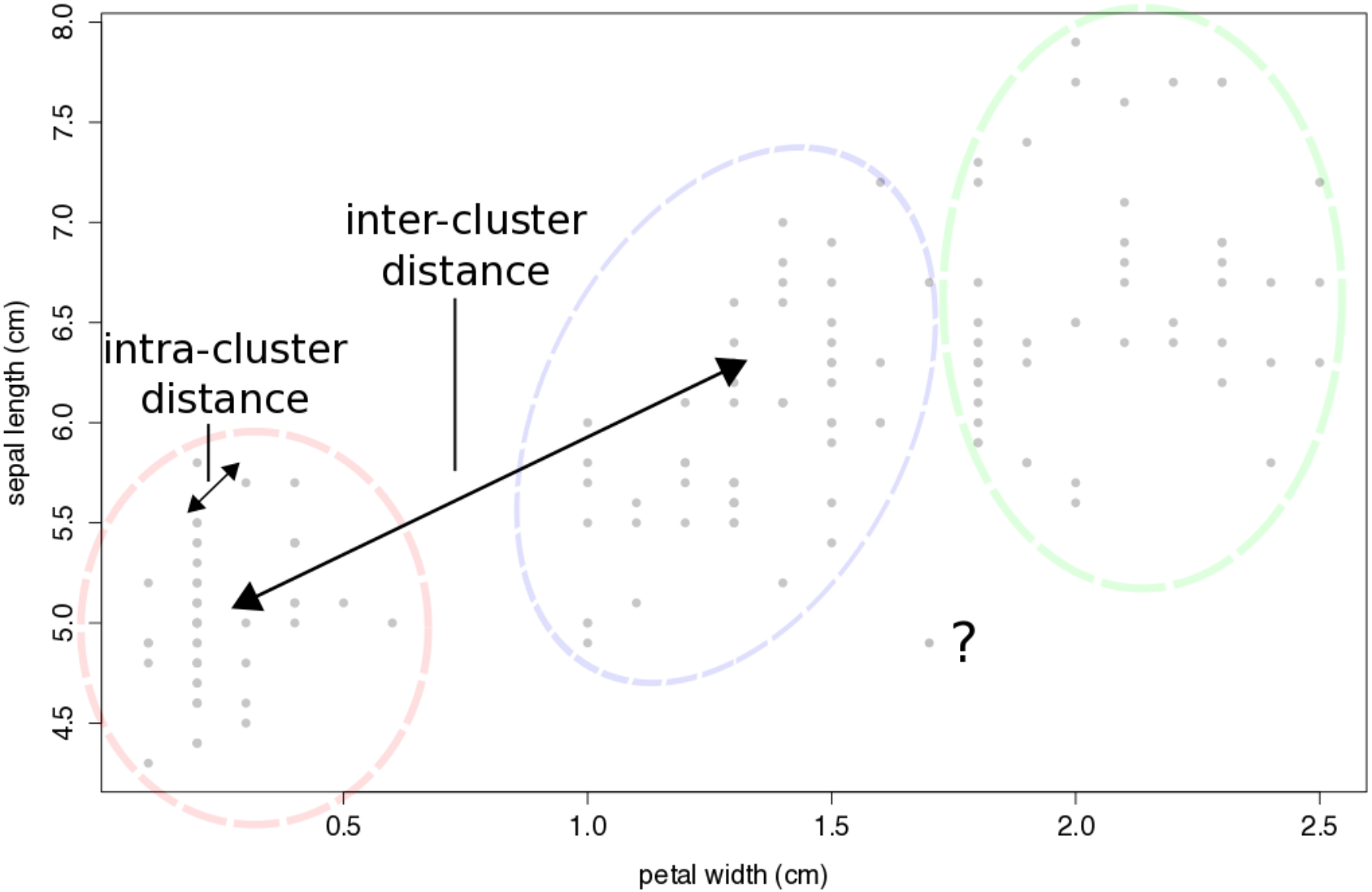
# What are we after?

Motivation: How is the data structured? Any outliers?

Goals: *High* intra-cluster similarity and *low* inter-cluster similarity



# Major types of clustering methods

**Partitional:** The data (feature) space is partitioned into $k$ regions

**Hierarchical:** Iteratively merging small clusters into larger ones (*agglomerative*) or breaking large clusters into smaller ones (*divisive*)

**Distribution-based:** Fit $k$ multivariate statistical distributions

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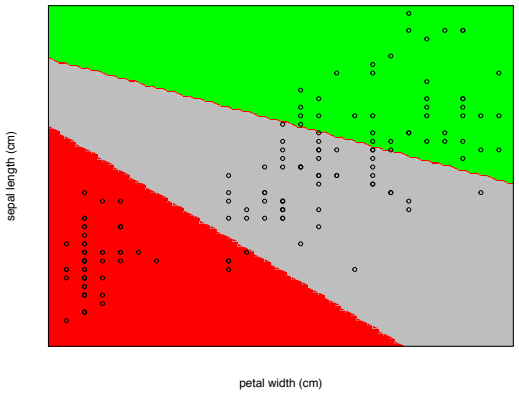


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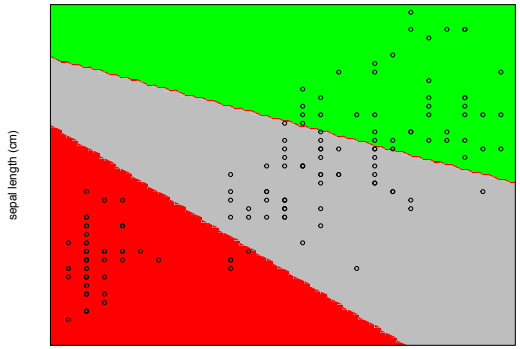


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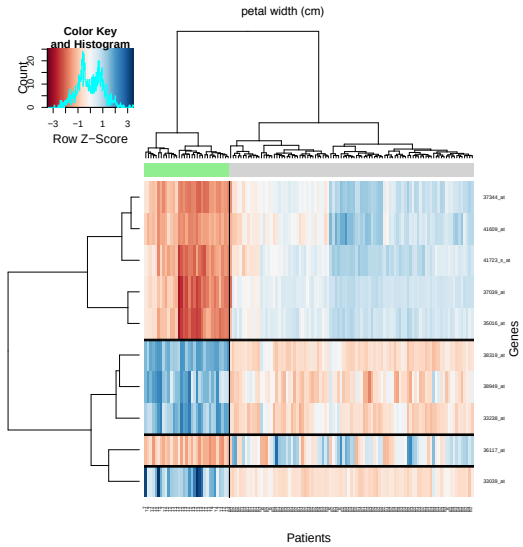


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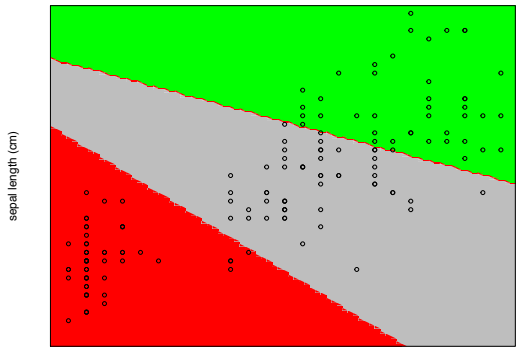


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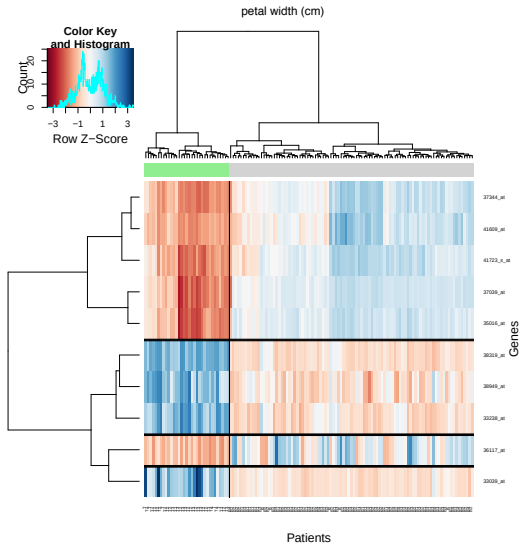


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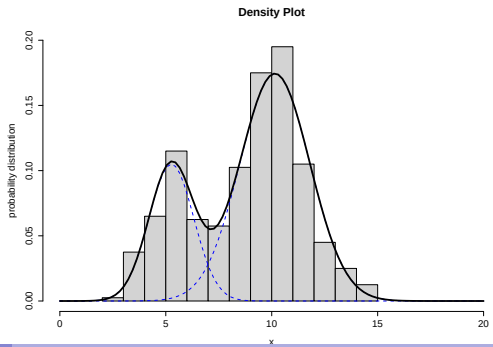
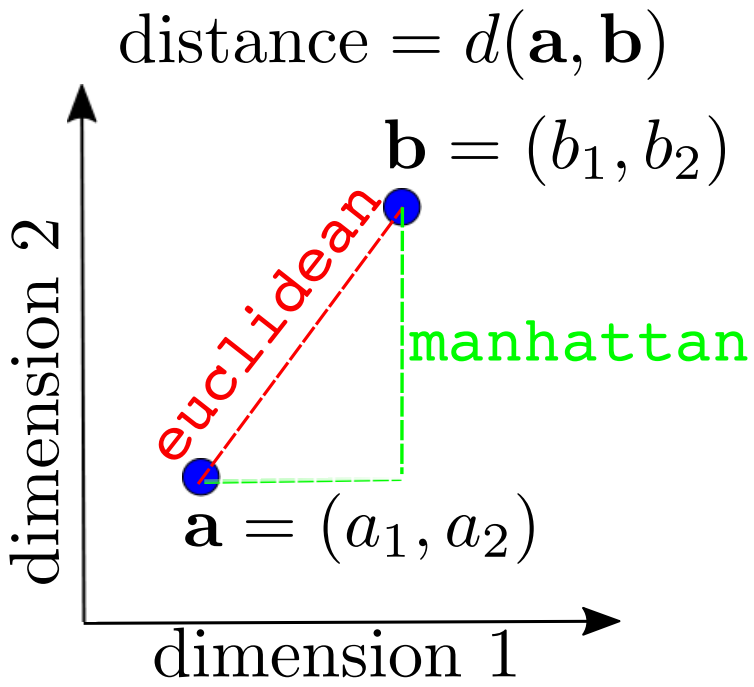


# Similarity measures

- A *distance* metric quantifies how *close* two data points are
- Several ways to define this distance which has a direct impact on the clustering result



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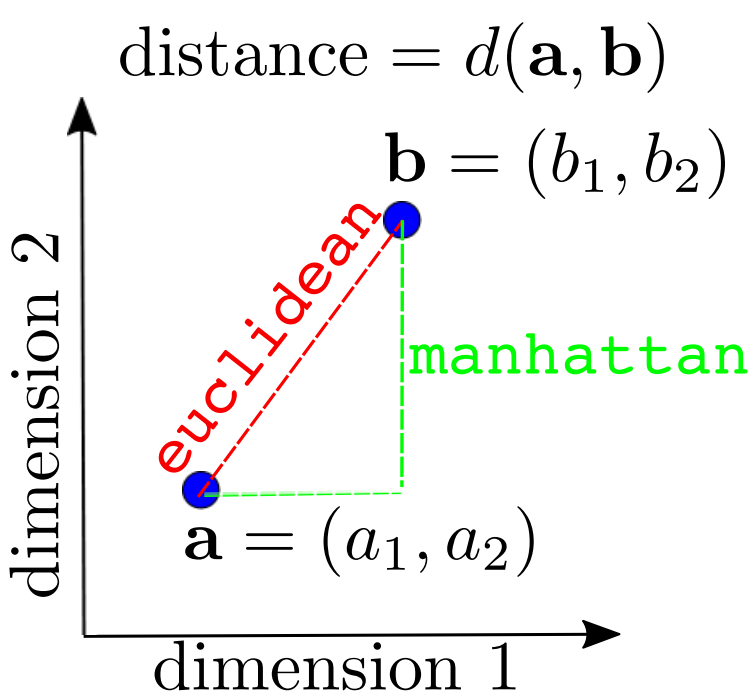


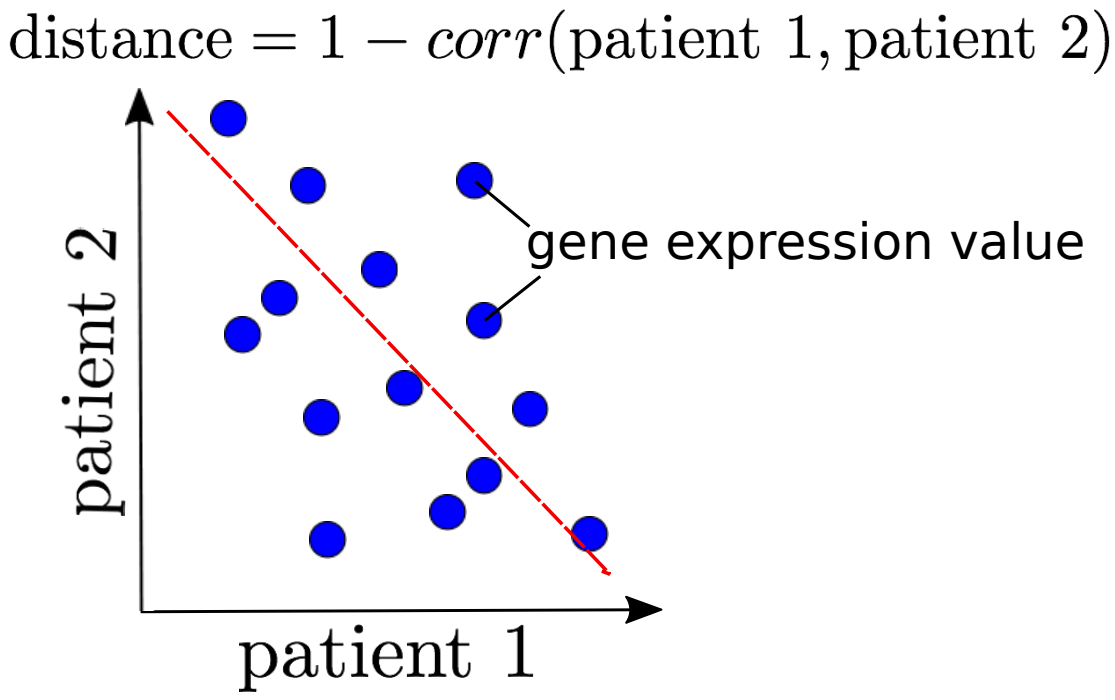

# $k$-means clustering

```
fit <- kmeans(x, centers)
# x - numeric matrix of data
# centers - no. of clusters k
```

1. Select $k$ centroids at random
2. Calculate distance between centroids and each data point
3. Assign each data point to the closest centroid
4. Compute new centroids; the average of all data points in that cluster
5. Repeat steps 2 to 4 until data points remain in the same cluster or some maximum number of iterations reached

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**Note**: $k$-means clustering should *only* be used with continuous data

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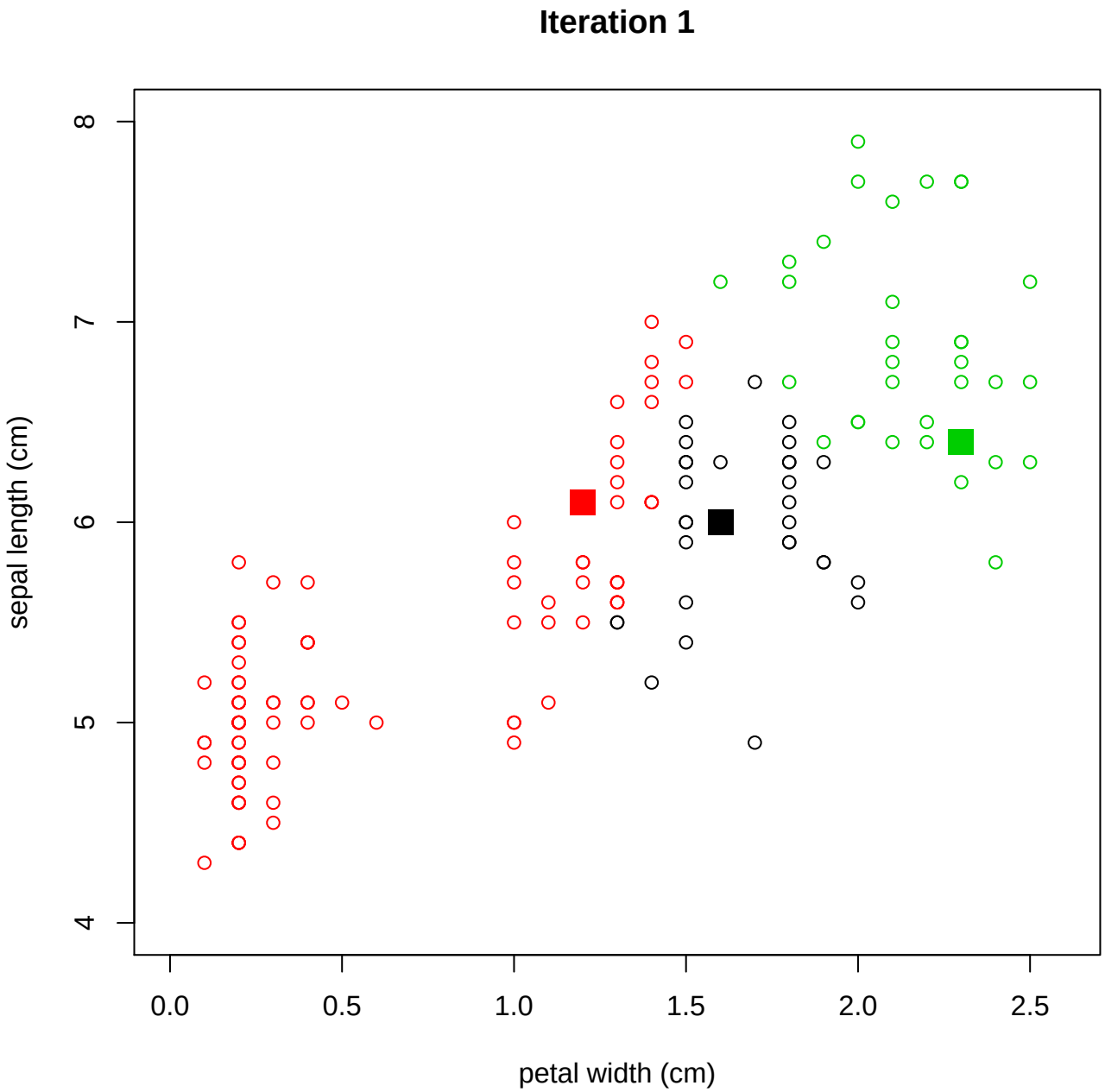

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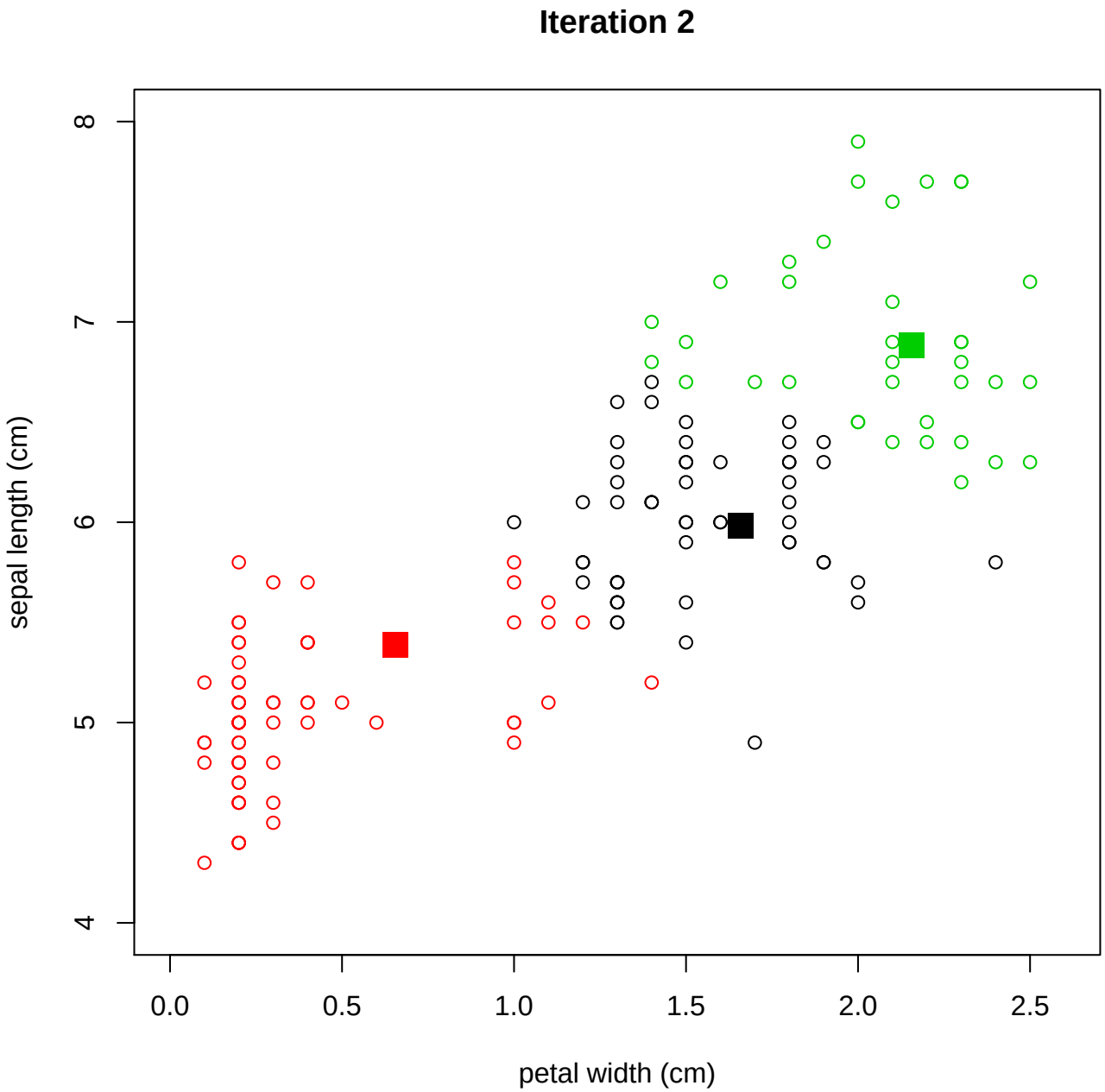

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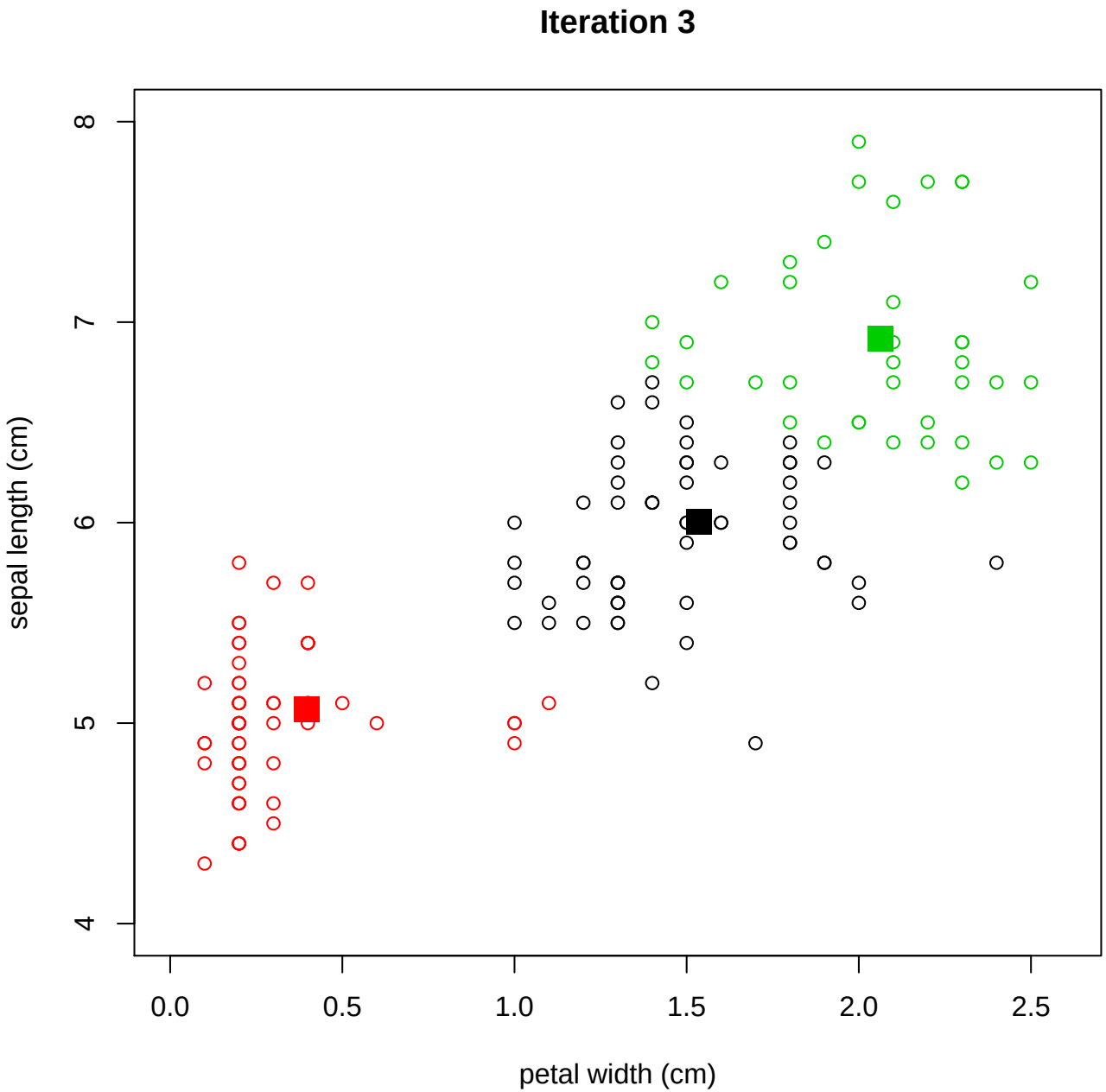

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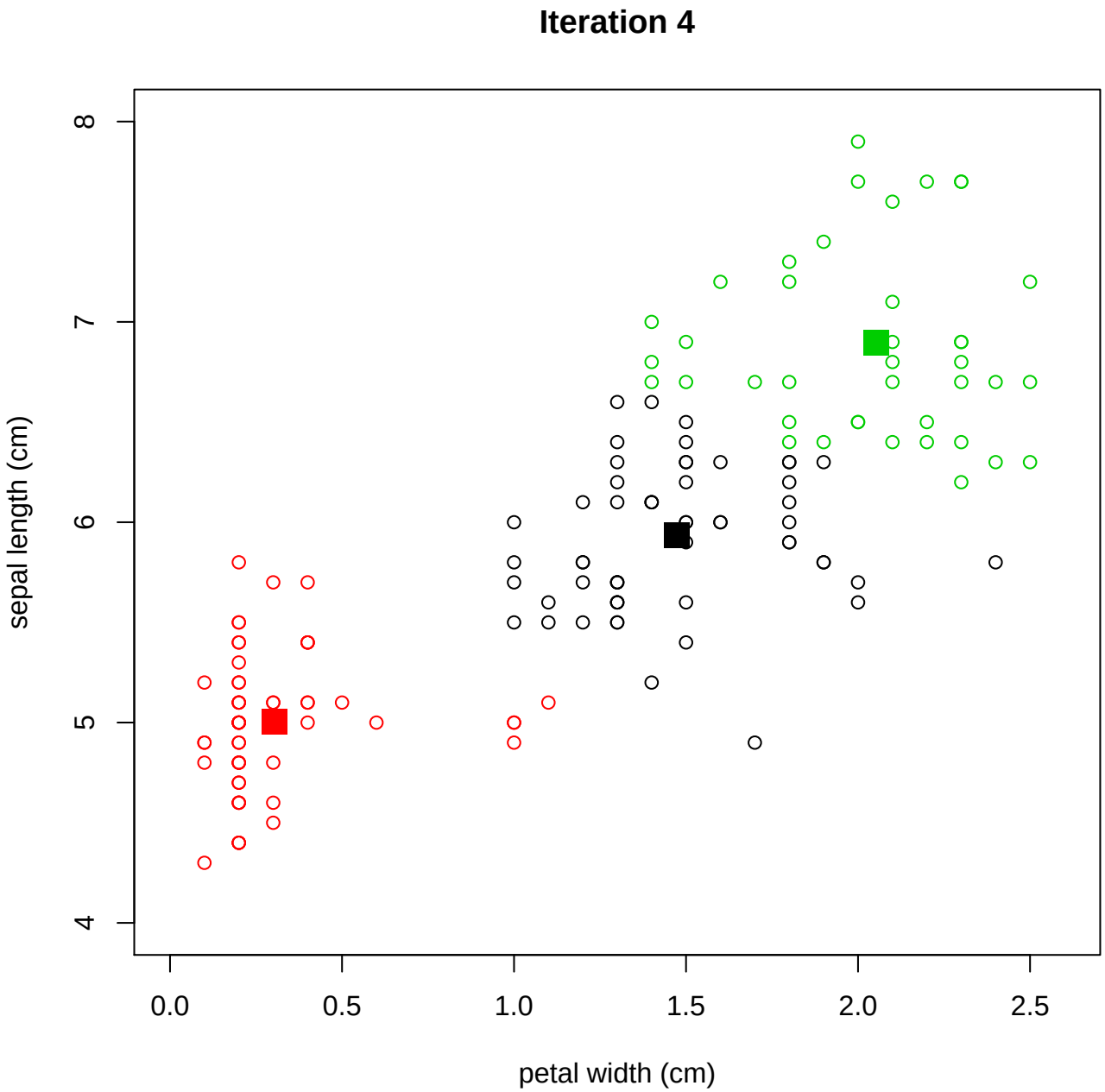

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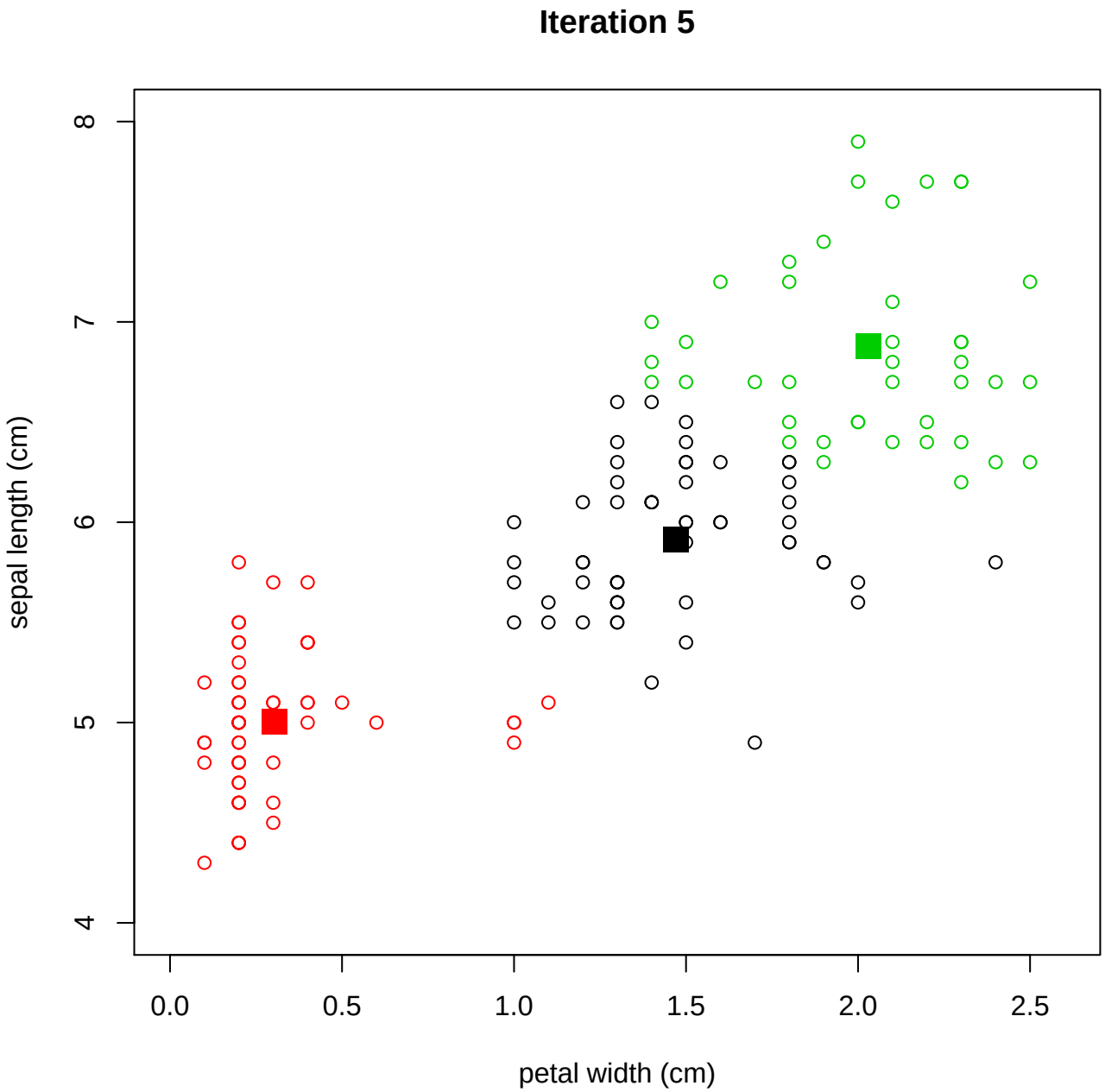

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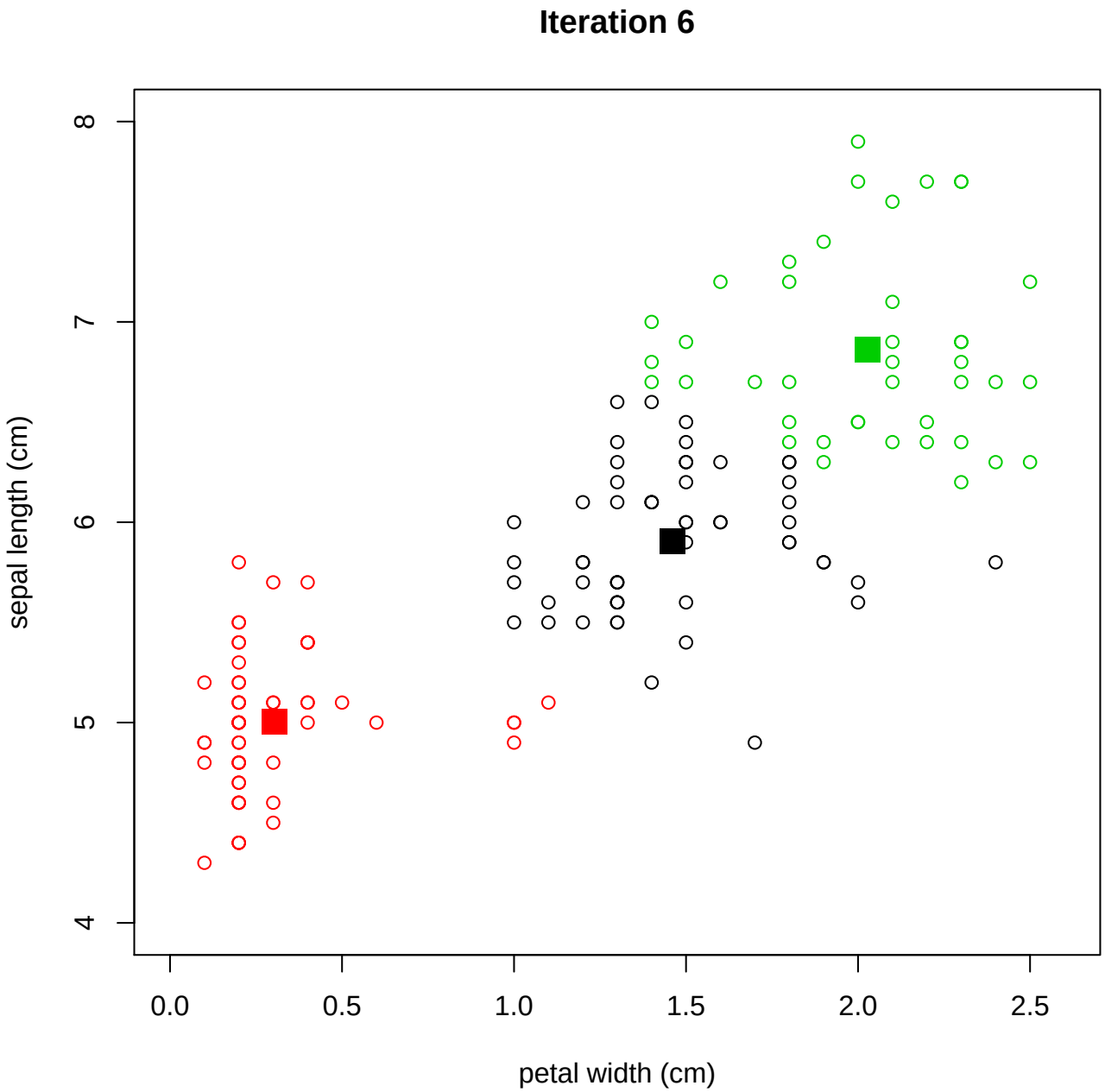

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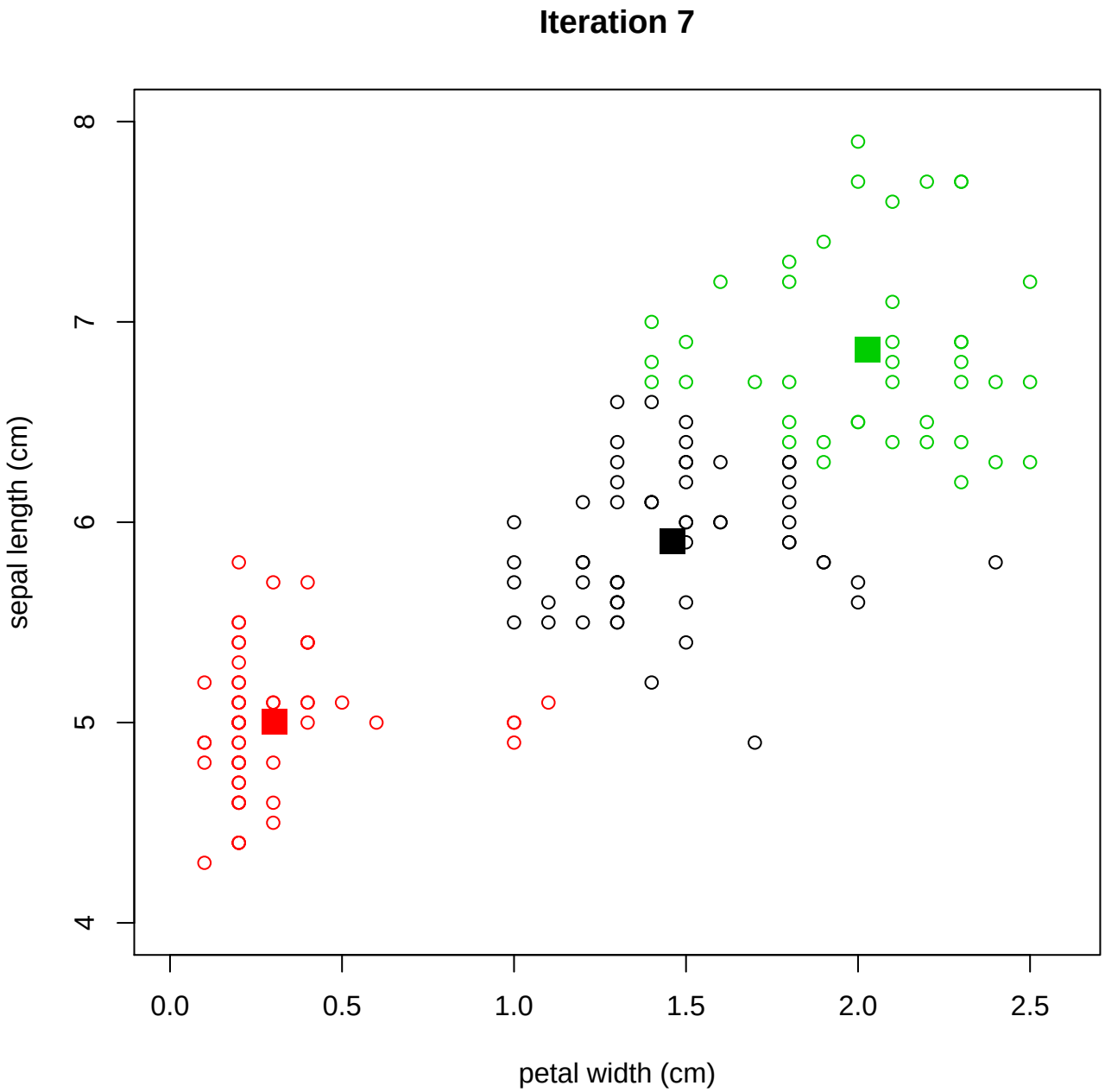

# $k$-means clustering

## Pros

- Simple and intuitive
- Computationally inexpensive/fast

## Cons

- What is $k$?
- Only applicable to continuous data where a mean is defined
- No guarantee of a global optimum solution

# Agglomerative hierarchical clustering

```
d <- dist(as.matrix(data), method)
# data - data frame
# method - distance method e.g "euclidean" or "manhattan"
fit <- hclust(d, method)
# method - linkage function e.g "complete" or "single"
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1. Assign each data point as its own cluster
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**Note**: Step 3 is *key*, the distance method and linkage function dictate the final result

# Hierarchical clustering: Link method

How do we compute the inter-cluster distance? The *linkage function*

Centroid: mean of data points (same as in $k$-means)

Single: distance between closest pair of points

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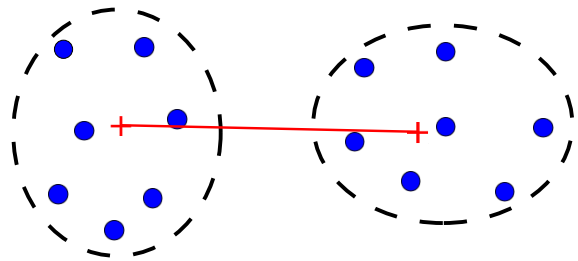

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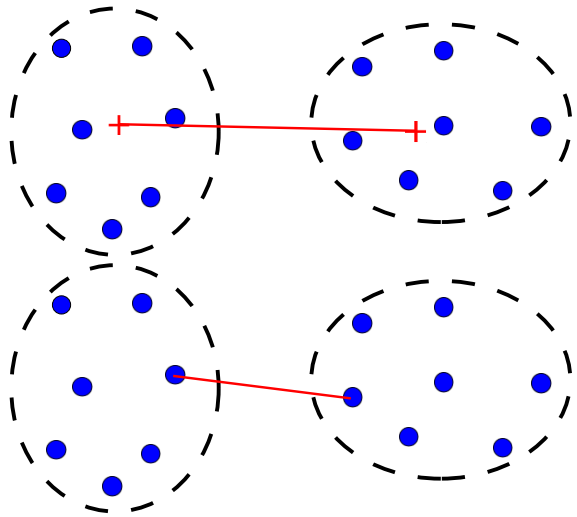

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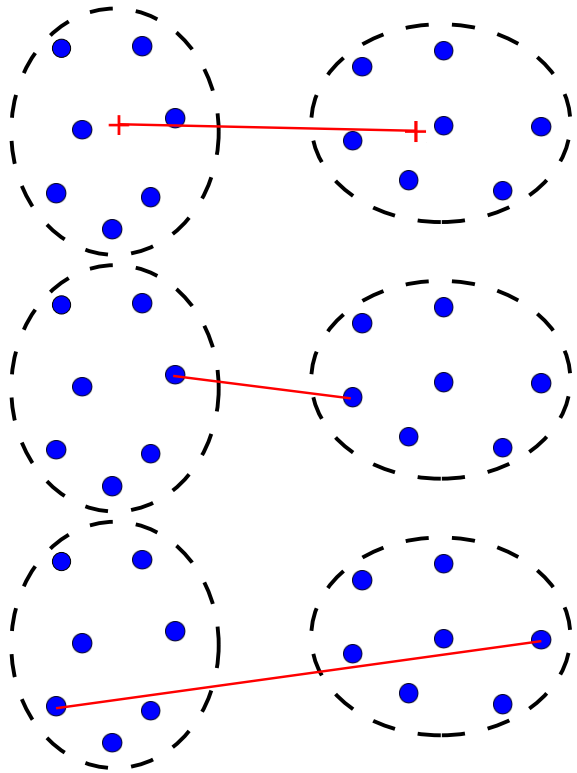

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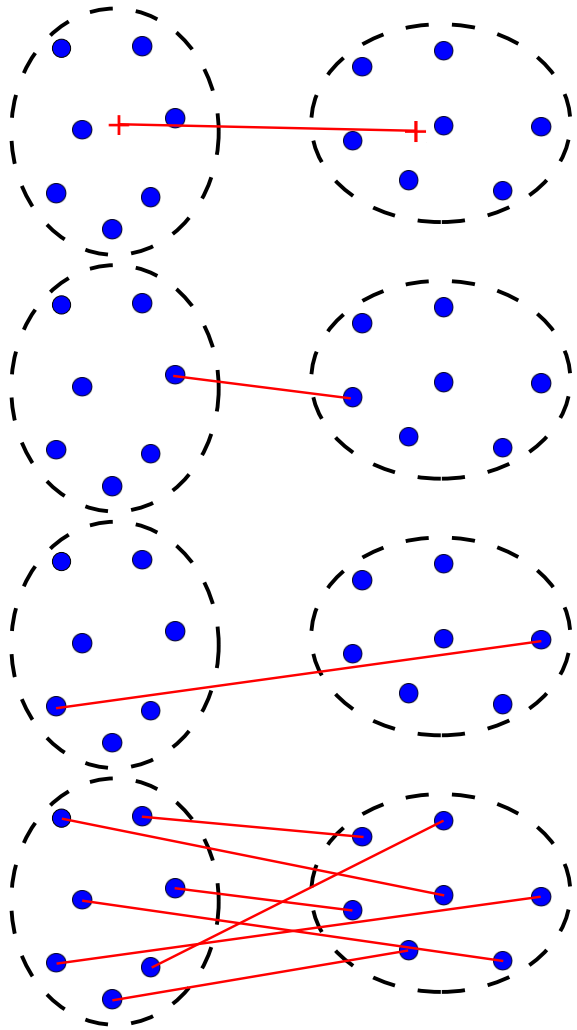
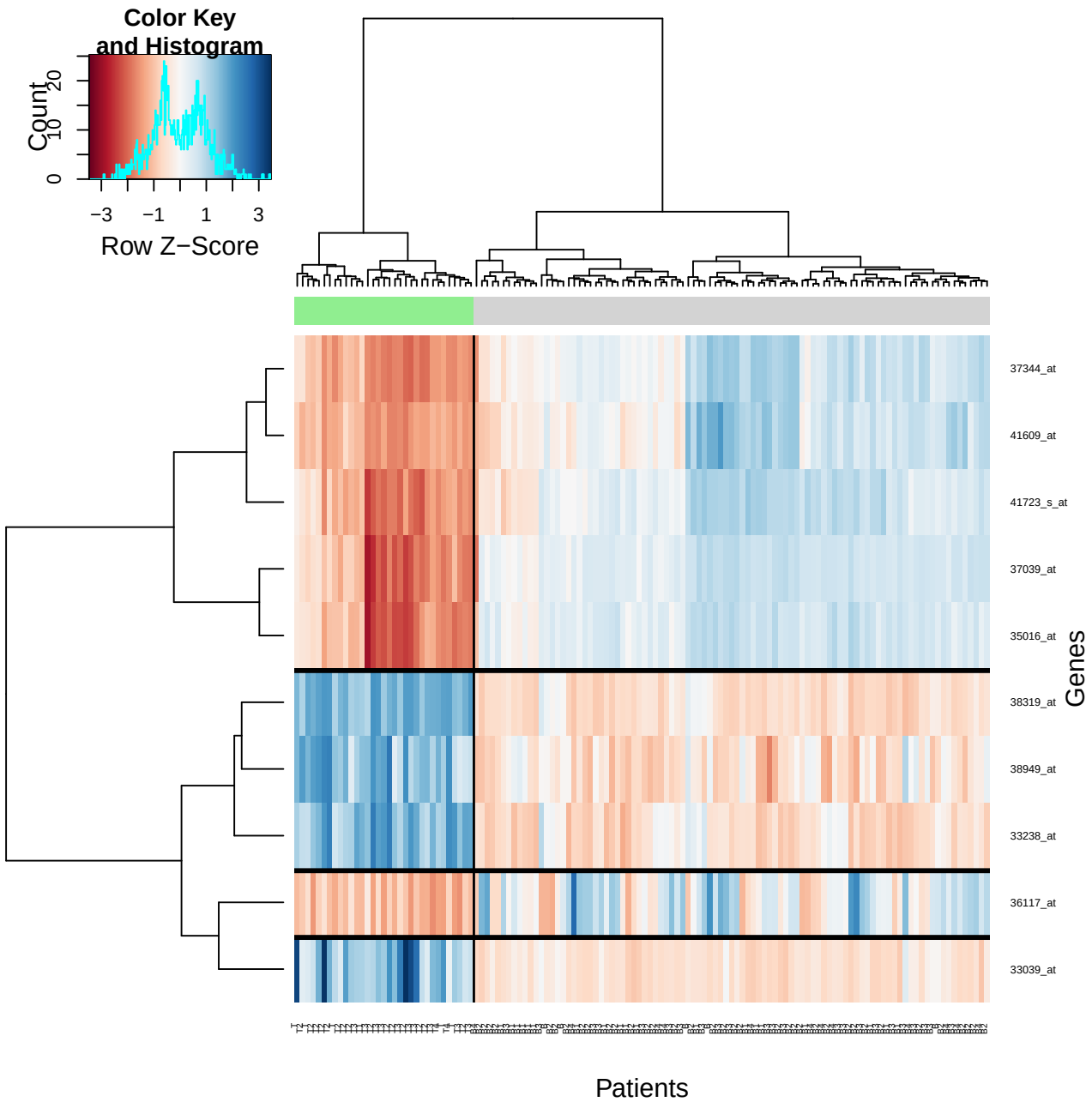


# Hierarchical clustering in gene expression studies



# Hierarchical clustering

## Pros

- No need to specify $k$
- Results can be visualised nicely irrespective of number of dimensions

## Cons

- Can be computationally expensive
- Interpretation is subjective. Where should we draw the line (to separate clusters)?
- Choice of distance method and linkage function can significantly change the result

# Gaussian mixture models

```
library(mclust)
fit <- Mclust(data, G)
# data - data frame
# G - no. of Gaussians
```

1. Fit $k$ multivariate Gaussian distributions

The Expectation-Maximisation (EM) algorithm is used to estimate the parameters $\pi_i$ (mixing coefficients), $\mu_i$ and $\sigma_i$

$$p(x) = \sum_{i=1}^{k} \pi_i \mathcal{N}(x|\mu_i, \Sigma_i) \text{ and } \sum_{i=1}^{k} \pi_i = 1$$

Can be seen as a "soft" version of $k$-means because *every* point is part of *every* cluster but with varying levels of membership

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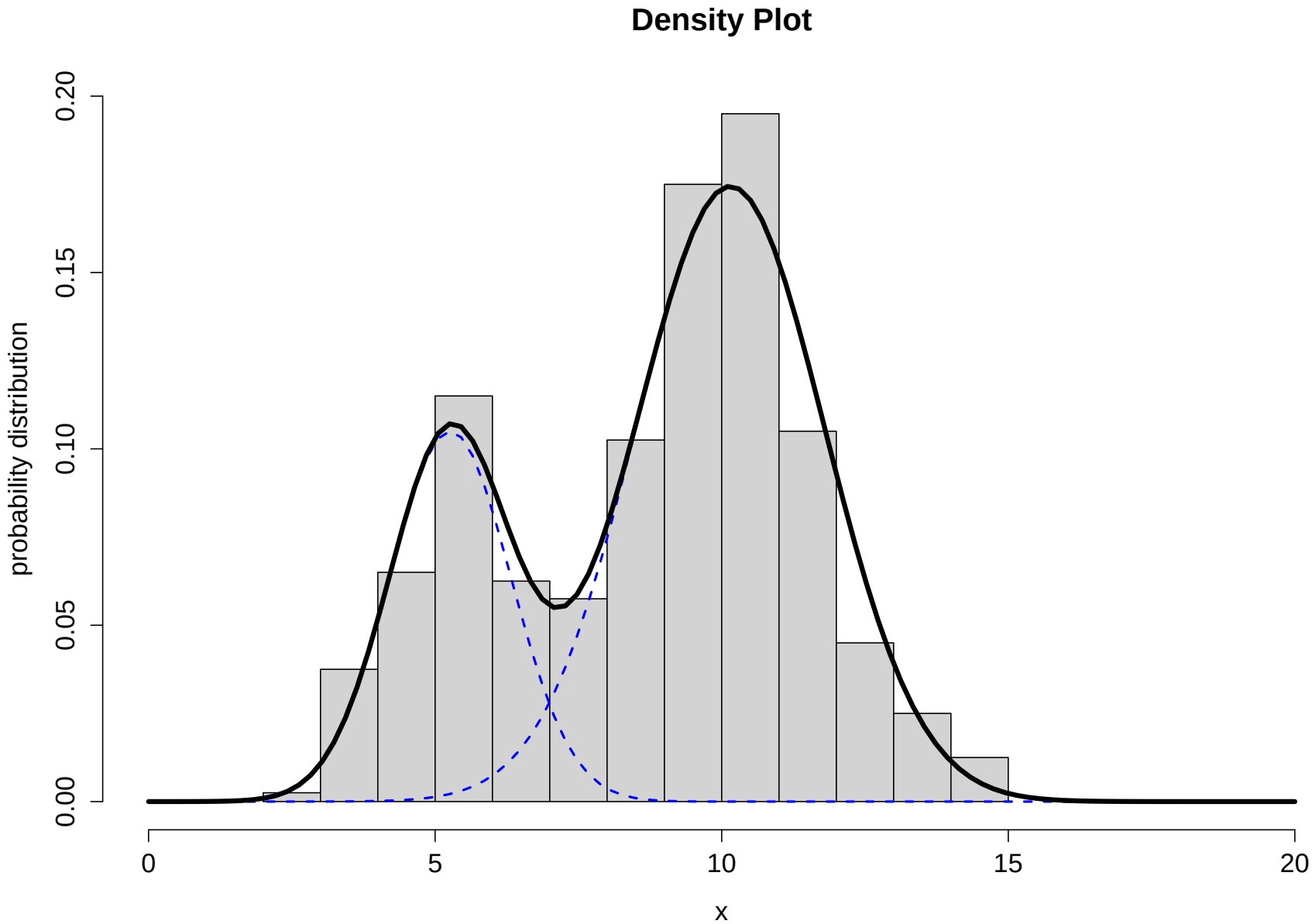

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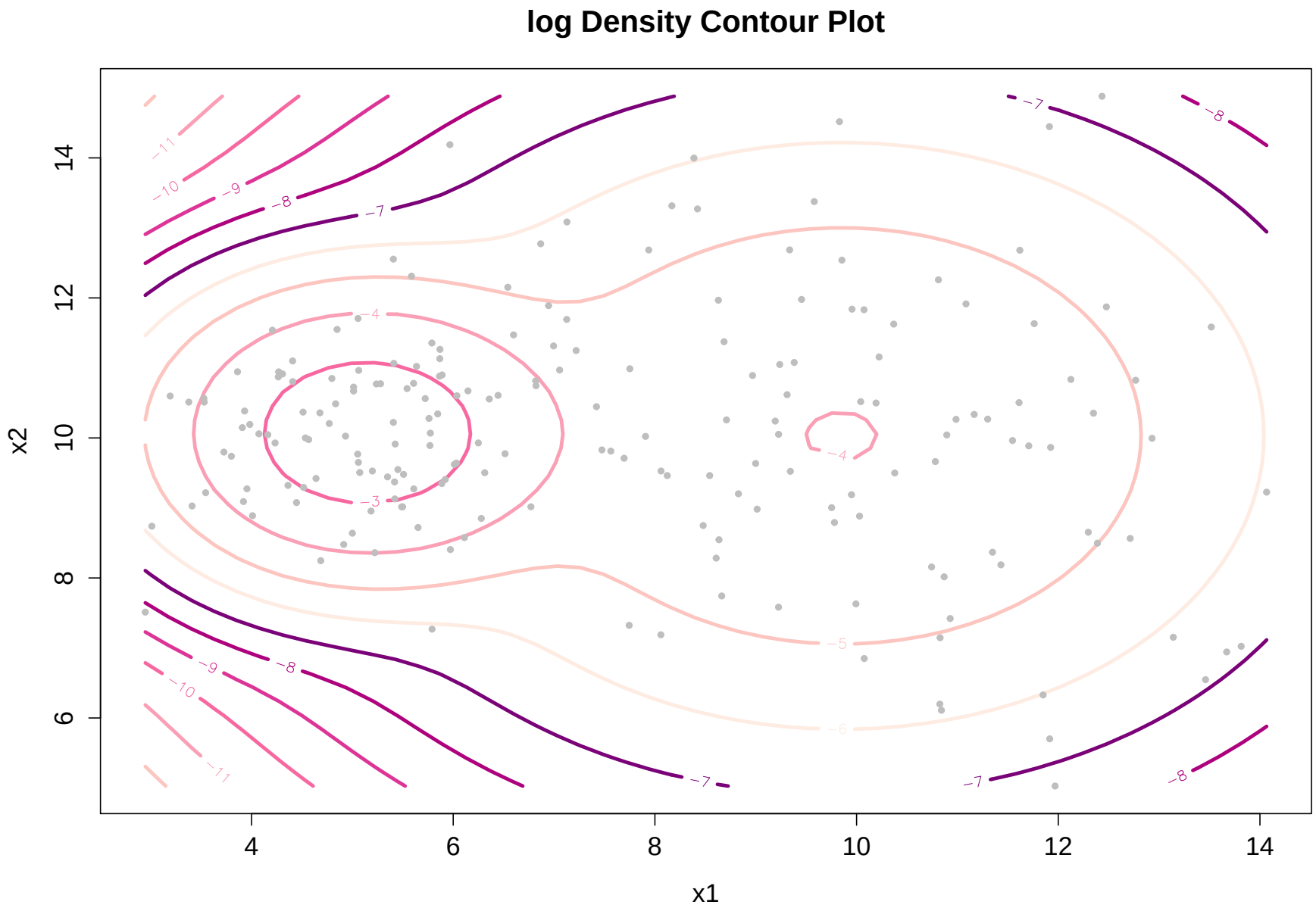

# Gaussian mixture models

## Pros

- Intuitive interpretation
- Computationally inexpensive

## Cons

- What is $k$?
- Strong assumption on the data (normality)
- No guarantee of a global optimum solution

# How do we determine the correct number of clusters?

**Short answer**: you can't

Because data is unlabelled the correct number of $k$ is ambiguous

However we can plot some indices as a function of $k$ to help us evaluate cluster validity:

- Within and between clusters sum-of-squares distances
- Akaike Information Criterion (AIC) or Bayesian Information Criterion (BIC) when using distribution-based methods
- Silhouette plot

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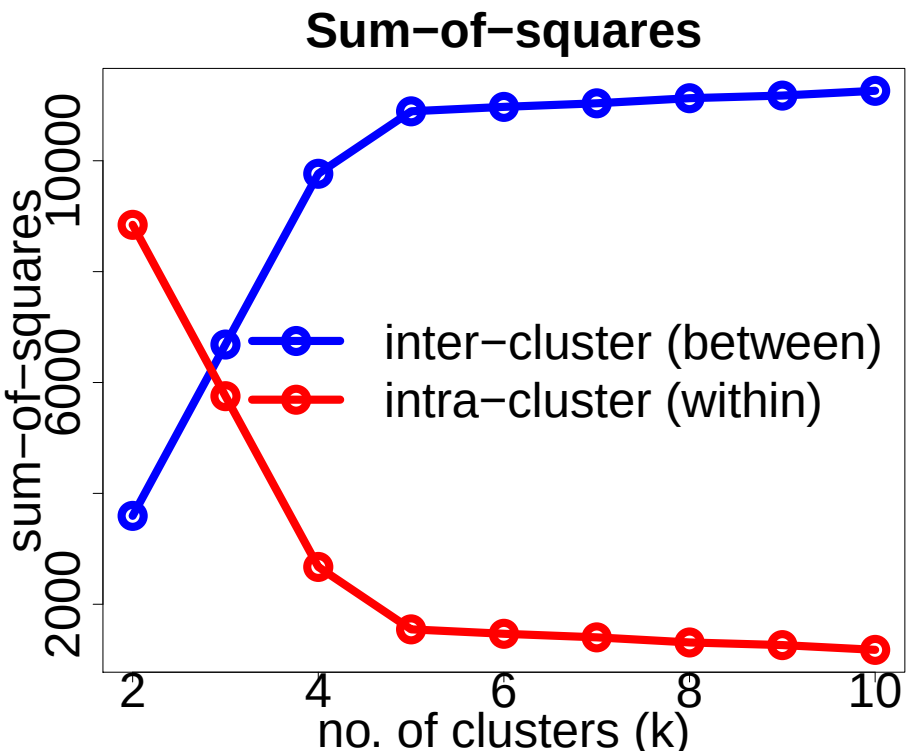


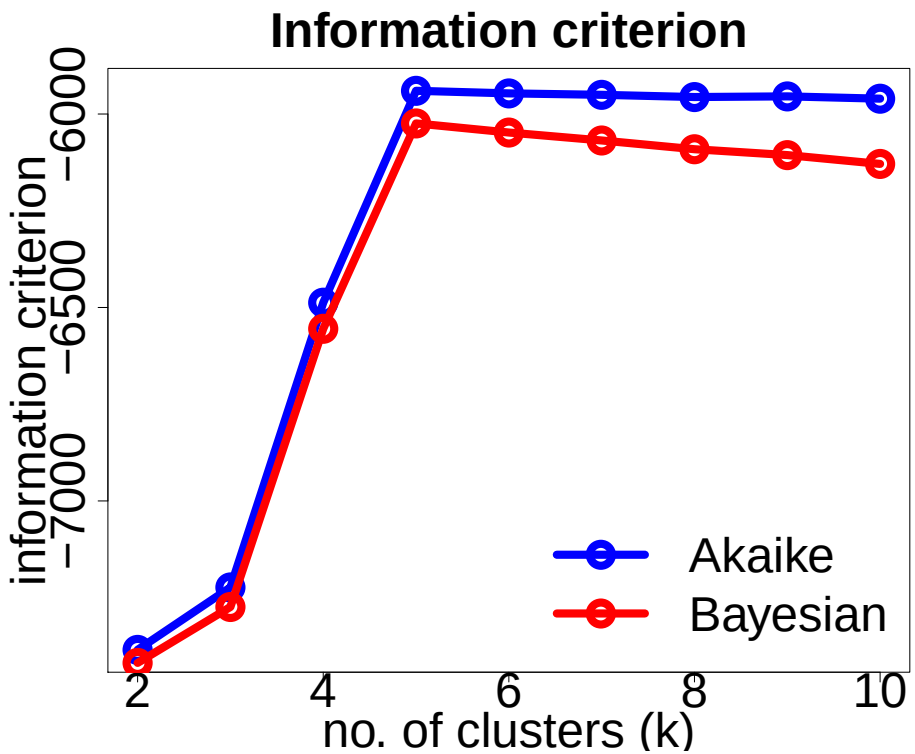

# How do we determine the correct number of clusters?

The `NbClust` package provides 30 different cluster validity metrics. A majority vote can be taken to deduce the appropriate number of clusters

```
library(NbClust)
NbClust(data, distance, method, min.nc, max.nc, index)
# data - data frame
# distance - similarity measure e.g "euclidean"
# method - clustering algorithm e.g "kmeans"
# min.nc - min number of clusters to consider
# max.nc - max number of clusters to consider
# index - which indices to compute, "all" computes all of them
```

**Note**:

- Indices *only* give us a ballpark range for "correct" number of clusters
- **Are they biologically relevant? Does it make sense? Prior knowledge to the rescue**
- E.g how many different phenotypes are you expecting?